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LETTER TO THE EDITOR

Transfer matrix algorithm for convection-biased diffusion

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Abstract. We present a novel transfer matrix algorithm to study convection-biased diffusion on a lattice. Average and mean-square exit time on two examples are discussed, one with uniform permeability and another with a log-uniform distribution. Different regimes (pure convection, pure diffusion, intermediate stage) are clearly identified.

Diffusion on random and fractal structures is a subject of high current interest, which has recently been extensively studied [1-6]. Some light has been shed on the interplay of the stochastic nature of the diffusion process and the randomness of the underlying physical system. More recently, biased diffusion has motivated a renewal of this interest. Basically, two types of bias can be considered, each having its own field of relevance.

(a) *Uniform bias*: the diffusion process is everywhere modified in the same way. This case is encountered when a uniform electric field is imposed on a domain where charged particles undergo Brownian motion, or in particle filtration where the gravity effects are important [7].

(b) *Local hydrodynamic bias*: the bias field depends on the disorder of the medium. This case is typical of dispersion problems where diffusion struggles against (or conspires with) convection, and consequently where different particles take different times to traverse the same distance. The latter is dictated by the hydrodynamics, which is a function of the detailed geometry and disorder. Other kinds of bias have been considered: random local bias where the diffusion process on a regular lattice is biased by a locally random field [3], chemical distance bias, which can be thought of as a simplification of the second case [8]; and so on.

In this letter, we address case (b) with a novel, exact, transfer matrix algorithm (equally applicable to any of the above-mentioned cases). We obtain the average and mean-square exit time for dispersion on a square lattice over a wide range of Peclet number, choosing a square lattice with bonds either parallel or perpendicular to the mean flow direction, which displays diffusive and convective regimes whenever disorder is present, as well as the pathological 'Wheatstone bridge' behaviour [9] in the perfectly ordered case. Our approach is similar in its physical content to that of a recent paper by de Arcangelis *et al* [5] who have treated, using an iterative algorithm, the case of a square lattice with '45° flow' which does not display the 'pathological' regime.

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For each elementary bond of our lattice we want to solve the convection-diffusion equation

$$\mathrm{d}\boldsymbol{C}/\mathrm{d}t = \partial \boldsymbol{C}/\partial t + u\,\partial \boldsymbol{C}/\partial x = D\,\partial^2 \boldsymbol{C}/\partial x^2 \tag{1}$$

which may also be written, defining a particle flux $\boldsymbol{j}(x, t) = u\boldsymbol{C} - D\,\partial \boldsymbol{C}/\partial x$, in the form of a conservation law: $\partial \boldsymbol{C}/\partial t + \partial \boldsymbol{j}/\partial x = 0$. Here $\boldsymbol{C}(x, t)$ represents the concentration of tracer particles, u is the velocity of the fluid moving in the bond (in the positive x direction) and D represents a molecular diffusion constant. At each node, $\boldsymbol{C}(x, t)$ is continuous and the total flux of particles is conserved. Taking the Laplace transform of (1) (assuming the channel originally empty), we obtain

$$sC(x, s) + u\,\mathrm{d}C(x, s)/\mathrm{d}x - D\,\mathrm{d}^2C(x, s)/\mathrm{d}x^2 = 0 \tag{2}$$

where s is the usual complex frequency. The solution of this equation is $C(x, s) = A\,\mathrm{e}^{\alpha x} + B\,\mathrm{e}^{\beta x}$, with $\alpha = [u + (u^2 + 4sD)^{1/2}]/2D$, and $\beta = [u - (u^2 + 4sD)^{1/2}]/2D$. The outward flux at the downstream end of the channel ($x = l$) is $j(l, t)$ whereas at the upstream end ($x = 0$) the outward flux is $-j(0, t)$. The linearity of equation (2) and the particle conservation law imply a linear dependence of $\{-j(0, s), j(l, s)\}$ on $\{C(0, s), C(l, s)\}$. In other words, we obtain in the transform space s a set of linear, non-symmetric equations relating at each node the conserved currents j to the concentrations C. This achieves the exact discretisation of the lattice. More precisely, this relation may be written in matrix form as

$$\begin{pmatrix} -j(0, s) \\ j(l, s) \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} C(0, s) \\ C(l, s) \end{pmatrix} \tag{3}$$

with $a = (\beta\,\mathrm{e}^{\beta l} - \alpha\,\mathrm{e}^{\alpha l})/(\mathrm{e}^{\alpha l} - \mathrm{e}^{\beta l})$, $b = (\alpha - \beta)/(\mathrm{e}^{\alpha l} - \mathrm{e}^{\beta l})$, $c = (\alpha - \beta)\,\mathrm{e}^{(\alpha+\beta)l}/(\mathrm{e}^{\alpha l} - \mathrm{e}^{\beta l})$ and $d = (\beta\,\mathrm{e}^{\alpha l} - \alpha\,\mathrm{e}^{\beta l})/(\mathrm{e}^{\alpha l} - \mathrm{e}^{\beta l})$. The ends of the channel can be thought of as sinks or sources of particles responding precisely to specified concentrations. A pulse response can be obtained by setting $j(0, s) = 1$ (equivalent to $\boldsymbol{j}(0, t) = \delta(t)$) and $C(l, s) = 0$ (sink condition). This formulation can be compared to the usual case of electrical conduction where, if V is the potential and i the current, then for one bond of conductance g Kirchhoff's laws yield a coupled symmetric set of equations

$$\begin{pmatrix} -i(0) \\ i(l) \end{pmatrix} = \begin{pmatrix} g & -g \\ -g & g \end{pmatrix} \begin{pmatrix} V(0) \\ V(l) \end{pmatrix}. \tag{4}$$

The matrix representation allows the use of a transfer matrix algorithm [10] to solve the problem of dispersion for the entire lattice with any kind of boundary conditions at the external modes. For a given s, the calculations are almost as easy as in the case of electrical conduction (though the matrices involved are not symmetric). If we are interested in the real-time response, we can proceed with the calculation for a number of values of s, and evaluate numerically the inverse Laplace transform of the function obtained. (This may be achieved with a fast-Fourier-transform program [11].)

Another result of significant interest is the calculation of various moments of the exit-time distribution. If $r(t)$, the exit-flux response of the system, corresponding to a pulse (delta function) input flux, has a Laplace transform $R(s)$, then

$$\langle t^N \rangle = \int_0^\infty t^N r(t)\,\mathrm{d}t = (-1)^N\,\mathrm{d}^N R(s)/\mathrm{d}s^N\big|_{s=0} \tag{5}$$

since $R(0)=1$ as a result of the conservation of particle flux. Thus, if we formally expand every quantity of interest up to the Nth order in s, and treat algebraically the different coefficients, then in one sweep through the lattice, our method yields the first N moments *exactly* without approximation.

We have investigated the pulse response of a square lattice, the bonds of which are either parallel or perpendicular to the mean flow direction. The local flow velocity (u previously) is first computed assuming linear permeability (Darcy's law). We consider the cases where the permeability of each bond is either constant (uniform throughout the whole lattice) or randomly distributed according to a log-uniform law. (The resultant velocities are proportional to the electrical currents that would flow in the bonds of an identical lattice with conductances corresponding to the above distribution of permeabilities.)

A dimensionless parameter, the so-called Peclet number Pe, can be introduced to describe the relative importance of convection and diffusion; ignoring any prefactors, it is dimensionally the ratio of a diffusion time (l^2/D) to a convection time (l/U):

$$Pe = Ul/D \tag{6}$$

where U is some characteristic velocity, l the length of the system and D a diffusion coefficient. It can be shown [12] that the proper way to define the characteristic velocity U_{eff} in a macroscopic system is to perform a volume average (see below).

(a) *Homogeneous lattice.* When the network is perfectly homogeneous the situation is classically 'pathological'. The transport on the half of the bonds normal to the flow direction will always remain diffusive, as there is no convective current through them. We display in figures 1 and 2 the behaviour of the average exit time $\langle t\rangle$ and its mean square $\langle t^2\rangle$. We can understand the different regimes exhibited as follows.

A typical time for a particle to be convected through a channel of length l, with a local velocity u, is $\tau_{\text{conv}}=l/u$, whereas the diffusion time is $\tau_{\text{diff}}=l^2/2D$. In the discussion below, $\bar{\tau}$ will refer to time related to the whole $(n\times n)$ lattice and τ to elementary bonds. Therefore $\bar{\tau}_{\text{conv}}=n\tau_{\text{conv}}$ and $\bar{\tau}_{\text{diff}}=m\tau_{\text{diff}}$, where $m=n^2+(n-1)^2$ is

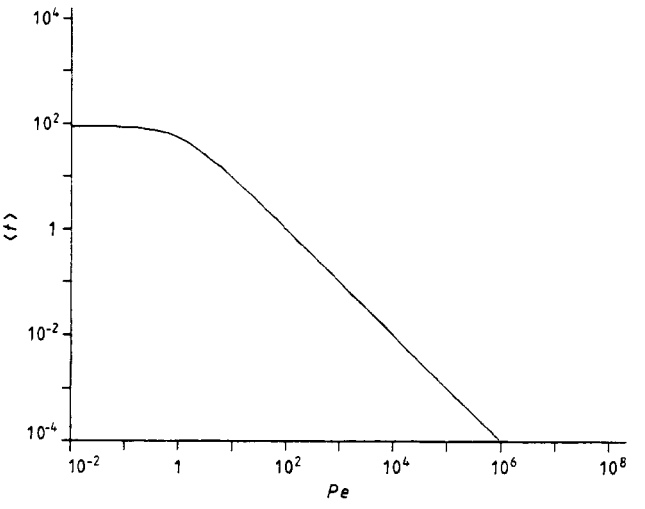

Figure 1. Log–log plot of the average exit time against macroscopic Peclet number for a homogeneous lattice. The curves corresponding to the disordered case (log-uniform distribution of permeabilities between 0.1 and 10) are indistinguishable on the scale of the figure.

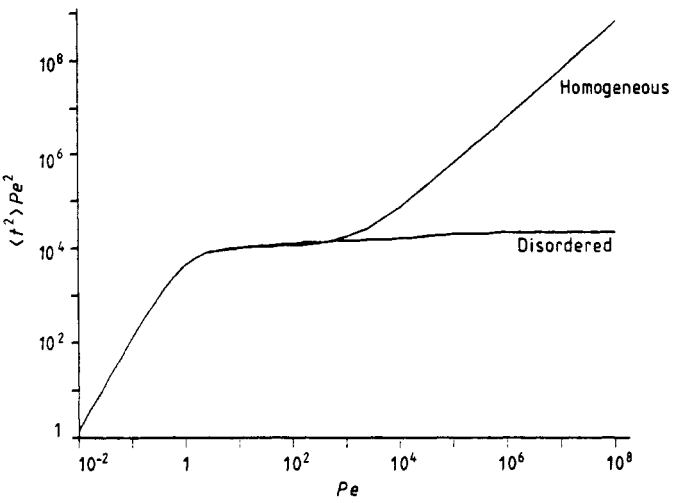

Figure 2. Log–log plot of the mean-squared exit time times squared Peclet number against Peclet number. In the homogeneous system the curve increases monotonically (with slope 1) for high Pe, whereas in the disordered case it reaches an asymptotic value.

the number of bonds in the lattice whenever $\bar{\tau}_{\text{diff}}$ is less than τ_{conv}, we can ignore convection. This holds when

$$l/u \gg ml^2/2D. \tag{7}$$

Recalling the global system variables, 'effective' velocity $U_{\text{eff}} = n^2u/m$ and macroscopic Peclet number $Pe = U_{\text{eff}}nl/D$, equation (7) implies

$$Pe \ll (U_{\text{eff}}/u)(2n/m) = 2n^3/m^2. \tag{8}$$

For the 10×10 lattice of figures 1 and 2, equation (8) gives $Pe \ll 0.06$. In this regime, $\langle t \rangle = ml^2/2D$ and $\langle t^2 \rangle = 5/3\langle t \rangle^2$. The effective diffusion constant is the molecular one. Transition to another regime occurs at a Peclet number Pe_1 when the convection and diffusion times for the whole lattice become comparable ($\bar{\tau}_{\text{conv}} = \bar{\tau}_{\text{diff}}$); then $nl/u = ml^2/2D$, i.e.

$$Pe_1 = (U_{\text{eff}}/u)(2n^2/m) = 2n^4/m^2. \tag{9}$$

A change of slope is clear in figures 1 and 2 for this crossover Peclet ($Pe_1 = 0.6$). For $Pe \gg Pe_1$, the average exit time $\langle t \rangle$ saturates and reaches the convective limit $\langle t \rangle = nl/U_{\text{eff}} = (n^2l^2/D)/Pe$. The situation is not as simple for the second moment $\langle t^2 \rangle$. In a qualitative way and for a high Peclet region, we can write any moment of the time distribution in the following form: a convective contribution for the whole network and a correction due to trapping in a diffusive arm. The probability of being trapped is

$$\varepsilon = (\text{number of diffusive arms per current line})(\tau_{\text{conv}}/\tau_{\text{diff}}). \tag{10}$$

For a high Peclet number, ε is much smaller than unity. This legitimises the approximation, which means that we neglect multiple trapping. We can therefore write

$$\langle t^N \rangle = (\bar{\tau}_{\text{conv}})^N(1-\varepsilon) + (\tau_{\text{diff}} + \bar{\tau}_{\text{conv}})^N\varepsilon. \tag{11}$$

We note that $\bar{\tau}_{conv}$ and ε vary as Pe^{-1} and τ_{diff} is independent of Pe. Keeping the dominant contributions in $\langle t \rangle$ and $\langle t^2 \rangle$, we obtain

$$\langle t \rangle = \bar{\tau}_{conv} + \tau_{diff}\varepsilon \sim Pe^{-1} \tag{12}$$

$$\langle t^2 \rangle = (\tau_{diff}^2 \varepsilon) \sim Pe^{-1}. \tag{13}$$

From (12) we see the correct scaling dependence as soon as $Pe \gg Pe_1$. The asymptotic form of $\langle t \rangle = nl/U_{eff}$ allows us to recover the expression for the effective velocity U_{eff}. If the first term, $\bar{\tau}_{conv}$, alone contributed, that would give an average only over the current-carrying part of the lattice. The trapping of particles in the dead arms modifies this 'velocity' and thanks to (10) we recover the volume average already quoted.

The expansion of (11) up to second order in Pe^{-1} gives

$$\langle t^2 \rangle = (\tau_{diff}^2 \varepsilon) + (\bar{\tau}_{conv}^2 + 2\tau_{conv}\tau_{diff}\varepsilon) \simeq (\tau_{diff}^2 \varepsilon) + (\bar{\tau}_{conv}^2). \tag{14}$$

This allows us to determine the 'crossover' Peclet number Pe_2 for which $\langle t^2 \rangle$ changes from a Pe^{-2} to a Pe^{-1} dependence, as the solution of $\varepsilon(Pe_2) \simeq \bar{\tau}_{conv}^2(Pe_2)/\tau_{diff}^2$. (In our case here, $Pe_2 \simeq 2000$.)

We have shown how the whole behaviour of $\langle t \rangle$ and $\langle t^2 \rangle$ is described for the homogeneous lattice. We can now turn to a less pathological situation in which a log-uniform distribution of permeabilities has been introduced.

(b) *Disordered lattice.* In this case, every bond carries a non-zero current. Therefore we will reach a purely convective regime if Pe is high enough. We show data again for a 10×10 lattice (though we have found similar behaviour for larger lattices as well). Even for a reasonably large distribution of permeabilities, G ($\log_{10} G$ uniformly distributed on $[-1, 1]$), the $\langle t \rangle$ data are almost indistinguishable from the previous case. The crossover Pe_1 has to be evaluated with averaged quantities, but as the distribution of $\log_{10} G$ is centred around the same value as before, and thanks to the definition of a global Peclet Pe, the numerical value of Pe_1 is unchanged.

The second moment $\langle t^2 \rangle$ is also very similar to that of the homogeneous lattice as long as $Pe \ll Pe_2$. This is understandable because only diffusion or first-moment convection times are required to describe these regions. But diffusion is the same in every bond and the first moment of the time distribution is relatively insensitive to disorder.

Between Pe_2 and another Peclet number Pe_3, we have a transition zone. Afterwards, $\langle t^2 \rangle$ becomes proportional to Pe^{-2} showing a convective dispersion. The distribution of exit times is then dictated by the transit time along all different downstream paths. Pe_3 is determined by the slowest of these paths. If the distribution of currents is broad, this slowest path is then controlled by the weakest current in one bond. So Pe_3 is given by the condition $l/u_{min} = l^2/2D$—i.e. $Pe_3 = 2U_{eff}/u_{min}$.

For the examples show in figures 1 and 2, $Pe_3 \simeq 10^5$. In the transition region, some bonds are diffusive. Equation (11) is still appropriate but now ε depends on Pe in a different way. ε takes into account the number of these diffusive traps and it varies with Pe, going to zero as Pe approaches Pe_3. We will discuss the general problem of the disordered lattice at greater length in a forthcoming paper.

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